Bifurcations and sudden current change in ensembles of classically chaotic ratchets

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In Phys. Rev. Lett. 84, 258 (2000), Mateos conjectured that current reversal in a classical deterministic ratchet is associated with bifurcations from chaotic to periodic regimes. This is based on the comparison of the current and the bifurcation diagram as a function of a given parameter for a periodic asymmetric potential. Barbi and Salerno, in Phys. Rev. E 62, 1988 (2000), have further investigated this claim and argue that, contrary to Mateos' claim, current reversals can occur also in the absence of bifurcations. Barbi and Salerno's studies are based on the dynamics of one particle rather than the statistical mechanics of an ensemble of particles moving in the chaotic system. The behavior of ensembles can be quite different, depending upon their characteristics, which leaves their results open to question. In this paper we present results from studies showing how the current depends on the details of the ensemble used to generate it, as well as conditions for convergent behavior (that is, independent of the details of the ensemble). We are then able to present the converged current as a function of parameters, in the same system as Mateos as well as Barbi and Salerno. We show evidence for current reversal without bifurcation, as well as bifurcation without current reversal. We conjecture that it is appropriate to correlate abrupt changes in the current with bifurcation, rather than current reversals, and show numerical evidence for our claims.

I. INTRODUCTION

The transport properties of nonlinear non-equilibrium dynamical systems are far from well-understood[1]. Consider in particular so-called ratchet systems which are asymmetric periodic potentials where an ensemble of particles experience directed transport[2, 3]. The origins of the interest in this lie in considerations about extracting useful work from unbiased noisy fluctuations as seems to happen in biological systems[4, 5]. Recently attention has been focused on the behavior of deterministic chaotic ratchets[6, 7, 8, 9, 10, 11] as well as Hamiltonian ratchets[12, 13].

Chaotic systems are defined as those which are sensitively dependent on initial conditions. Whether chaotic or not, the behavior of nonlinear systems – including the transition from regular to chaotic behavior – is in general sensitively dependent on the parameters of the system. That is, the phase-space structure is usually relatively complicated, consisting of stability islands embedded in chaotic seas, for examples, or of simultaneously co-existing attractors. This can change significantly as parameters change. For example, stability islands can merge into each other, or break apart, and the chaotic sea itself may get pinched off or otherwise changed, or attractors can change symmetry or bifurcate. This means that the transport properties can change dramatically as well. A few years ago, Mateos[7] considered a specific ratchet model with a periodically forced underdamped particle. He looked at an ensemble of particles, specifically the velocity for the particles, averaged over time

and the entire ensemble. He showed that this quantity, which is an intuitively reasonable definition of 'the current', could be either positive or negative depending on the amplitude a of the periodic forcing for the system. At the same time, there exist ranges in a where the trajectory of an individual particle displays chaotic dynamics. Mateos conjectured a connection between these two phenomena, specifically that the reversal of current direction was correlated with a bifurcation from chaotic to periodic behavior in the trajectory dynamics. Even though it is unlikely that such a result would be universally valid across all chaotic deterministic ratchets, it would still be extremely useful to have general heuristic rules such as this. These organizing principles would allow some handle on characterizing the many different kinds of behavior that are possible in such systems.

A later investigation[8] of the Mateos conjecture by Barbi and Salerno, however, argued that it was not a valid rule even in the specific system considered by Mateos. They presented results showing that it was possible to have current reversals in the absence of bifurcations from periodic to chaotic behavior. They proposed an alternative origin for the current reversal, suggesting it was related to the different stability properties of the rotating periodic orbits of the system. These latter results seem fundamentally sensible. However, this paper based its arguments about currents on the behavior of a *single* particle as opposed to an ensemble. This implicitly assumes that the dynamics of the system are ergodic. This is not true in general for chaotic systems of the type being considered. In particular, there can be ex-

treme dependence of the result on the statistics of the ensemble being considered. This has been pointed out in earlier studies [6] which laid out a detailed methodology for understanding transport properties in such a mixed regular and chaotic system. Depending on specific parameter value, the particular system under consideration has multiple coexisting periodic or chaotic attractors or a mixture of both. It is hence appropriate to understand how a probability ensemble might behave in such a system. The details of the dependence on the ensemble are particularly relevant to the issue of the possible experimental validation of these results, since experiments are always conducted, by virtue of finite-precision, over finite time and finite ensembles. It is therefore interesting to probe the results of Barbi and Salerno with regard to the details of the ensemble used, and more formally, to see how ergodicity alters our considerations about the current, as we do in this paper.

We report here on studies on the properties of the current in a chaotic deterministic ratchet, specifically the same system as considered by Mateos[7] and Barbi and Salerno[8]. We consider the impact of different kinds of ensembles of particles on the current and show that the current depends significantly on the details of the initial ensemble. We also show that it is important to discard transients in quantifying the current. This is one of the central messages of this paper: Broad heuristics are rare in chaotic systems, and hence it is critical to understand the ensemble-dependence in any study of the transport properties of chaotic ratchets. Having established this, we then proceed to discuss the connection between the bifurcation diagram for individual particles and the behavior of the current. We find that while we disagree with many of the details of Barbi and Salerno's results, the broader conclusion still holds. That is, it is indeed possible to have current reversals in the absence of bifurcations from chaos to periodic behavior as well as bifurcations without any accompanying current reversals.

The result of our investigation is therefore that the transport properties of a chaotic ratchet are not as simple as the initial conjecture. However, we do find evidence for a generalized version of Mateos's conjecture. That is, in general, bifurcations for trajectory dynamics as a function of system parameter seem to be associated with abrupt changes in the current. Depending on the specific value of the current, these abrupt changes may lead the net current to reverse direction, but not necessarily so.

We start below with a preparatory discussion necessary to understand the details of the connection between bifurcations and current reversal, where we discuss the potential and phase-space for single trajectories for this system, where we also define a bifurcation diagram for this system. In the next section, we discuss the subtleties of establishing a connection between the behavior of individual trajectories and of ensembles. After this, we are able to compare details of specific trajectory bifurcation curves with current curves, and thus justify our broader statements above, after which we conclude.

II. REGULARITY AND CHAOS IN SINGLE-PARTICLE RATCHET DYNAMICS

The goal of these studies is to understand the behavior of general chaotic ratchets. The approach taken here is that to discover heuristic rules we must consider specific systems in great detail before generalizing. We choose the same 1-dimensional ratchet considered previously by Mateos[7], as well as Barbi and Salerno[8]. We consider an ensemble of particles moving in an asymmetric periodic potential, driven by a periodic time-dependent external force, where the force has a zero time-average. There is no noise in the system, so it is completely deterministic, although there is damping. The equations of motion for an individual trajectory for such a system are given in dimensionless variables by

$$\ddot{x} + b\dot{x} + \frac{dV(x)}{dt} = a\cos(\omega t) \qquad (1)$$

where the periodic asymmetric potential can be written in the form

$$V(x) = C - \frac{1}{4\pi^2\delta}\left[\sin[2\pi(x-x_0)] + \frac{1}{4}\sin[4\pi(x-x_0)]\right]. \qquad (2)$$

In this equation C, x_0 have been introduced for convenience such that one potential minimum exists at the origin with $V(0) = 0$ and the term $\delta = \sin(2\pi|x_0|) + \frac{1}{4}\sin(4\pi|x_0|)$.

The phase-space of the undamped undriven ratchet – the system corresponding to the unperturbed potential $V(x)$ – looks like a series of asymmetric pendula. That is, individual trajectories have one of following possible time-asymptotic behaviors: (i) Inside the potential wells, trajectories and all their properties oscillate, leading to zero net transport. Outside the wells, the trajectories either (ii) librate to the right or (iii) to the left, with corresponding net transport depending upon initial conditions. There are also (iv) trajectories on the separatrices between the oscillating and librating orbits, moving between unstable fixed points in infinite time, as well as the unstable and stable fixed points themselves, all of which constitute a set of negligible measure.

When damping is introduced via the b-dependent term in Eq. 1, it makes the stable fixed points the only attractors for the system. When the driving is turned on, the phase-space becomes chaotic with the usual phenomena of intertwining separatrices and resulting homoclinic tangles. The dynamics of individual trajectories in such a system are now very complicated in general and depend sensitively on the choice of parameters and initial conditions. We show snapshots of the development of this kind of chaos in the set of Poincaré sections Fig. (1b,c) together with a period-four orbit represented by the center of the circles.

A broad characterization of the dynamics of the problem as a function of a parameter $(a, b$ or $\omega)$ emerges in a bifurcation diagram. This can be constructed in sev-
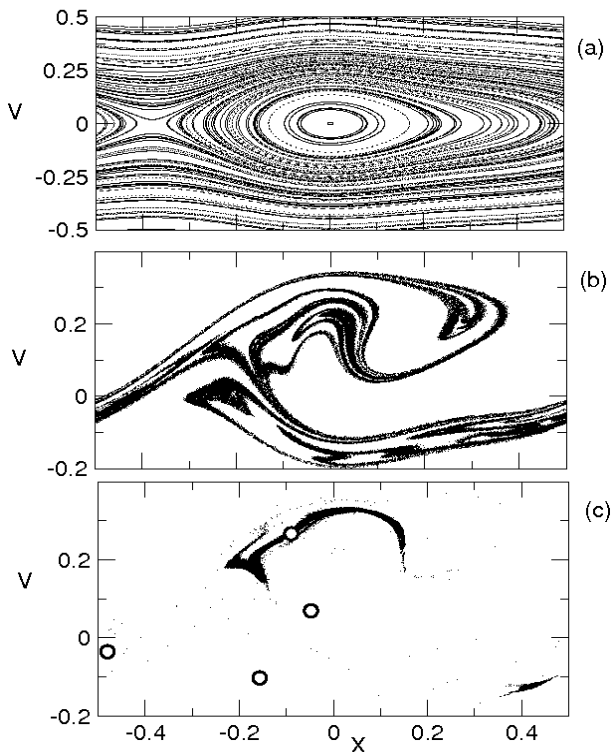
FIG. 1: (a) Classical phase space for the unperturbed system. For $\omega = 0.67$, $b = 0.1$, two chaotic attractors emerge with $a = 0.11$ (b) $a = 0.155$ (c) and a period four attractor consisting of the four centers of the circles with $a = 0.08125$.

eral different and essentially equivalent ways. The relatively standard form that we use proceeds as follows: First choose the bifurcation parameter (let us say a) and correspondingly choose fixed values of b, ω, and start with a given value for $a = a_{min}$. Now iterate an initial condition, recording the value of the particle's position $x(T_P)$ at times T_p from its integrated trajectory (sometimes we record $\dot{x}(T_P)$). This is done stroboscopically at discrete times $T_P = n_p * T_\omega$ where $T_\omega = \frac{2\pi}{\omega}$ and n_P is an integer $1 \leq n_P < M$ with M the maximum number of observations made. Of these, discard observations at times less than some cut-off time $n_c * T_\omega$ and plot the remaining points against a_{min}. It must be noted that discarding transient behavior is critical to get results which are independent of initial condition, and we shall emphasize this further below in the context of the net transport or current.

If the system has a fixed-point attractor then all of the data lie at one particular location x_c. A periodic orbit with period $j * T_\omega$ (that is, with period commensurate with the driving) shows up with $M - n_t$ points occupying only j different locations of x for a_{min}. All other orbits, including periodic orbits of incommensurate period result in a simply-connected or multiply-connected dense set of points. For the next value $a = a_{min} + da$, the last computed value of x, v at $a = a_{min}$ are used as initial conditions, and previously, results are stored after

cutoff and so on until $a = a_{min} + (j - 1) * da = a_{max}$. That is, the bifurcation diagram is generated by sweeping the relevant parameter, in this case a, from a_{min} through some maximum value a_{max}. This procedure is intended to catch all coexisting attractors of the system with the specified parameter range. Note that several initial conditions are effectively used troughout the process, and a bifurcation diagram is not the behavior of a single trajectory. We have made several plots, as a test, with different initial conditions and the diagrams obtained are identical. We show several examples of this kind of bifurcation diagram below, where they are being compared with the corresponding behavior of the current.

Having broadly understood the wide range of behavior for individual trajectories in this system, we now turn in the next section to a discussion of the non-equilibrium properties of a statistical ensemble of these trajectories, specifically the current for an ensemble.

III. ENSEMBLE CURRENTS

The current J for an ensemble in the system is defined in an intuitive manner by Mateos[7] as the time-average of the average velocity over an ensemble of initial conditions. That is, an average over several initial conditions is performed at a given observation time t_j to yield the average velocity over the particles

$$v_j = \frac{1}{N} \sum_{i=1}^{N} \dot{x}_i(t_j). \tag{3}$$

This average velocity is then further time-averaged; given the discrete time t_j for observation this leads to a second sum

$$J = \frac{1}{M} \sum_{j=1}^{M} v_j \tag{4}$$

where M is the number of time-observations made.

For this to be a relevant quantity to compare with bifurcation diagrams, J should be independent of the quantities N, M but still strongly dependent on a, b, ω. A further parameter dependence that is being suppressed in the definition above is the shape and location of the ensemble being used. That is, the transport properties of an ensemble in a chaotic system depend in general on the part of the phase-space being sampled. It is therefore important to consider many different initial conditions to generate a current. The first straightforward result we show in Fig. (2) is that in the case of chaotic trajectories, a single trajectory easily displays behavior very different from that of many trajectories. However, it turns out that in the regular regime, it is possible to use a single trajectory to get essentially the same result as obtained from many trajectories.

Further consider the bifurcation diagram in Fig. (3) where we superimpose the different curves resulting from

varying the number of points in the initial ensemble. First, the curve is significantly smoother as a function of a for larger N. Even more relevant is the fact that the single trajectory data ($N = 1$) may show current reversals that do not exist in the large N data.
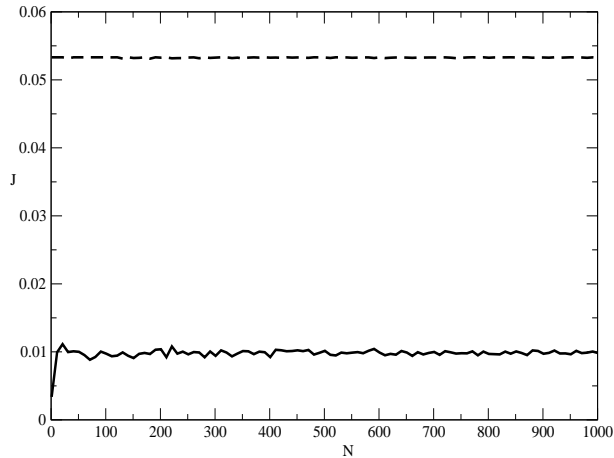

FIG. 2: Current J versus the number of trajectories N for $\omega = 0.67$; dashed lines correspond to a regular motion with $a = 0.12$ while solid lines correspond to a chaotic motion with $a = 0.08$. Note that a single trajectory is sufficient for a regular motion while the convergence in the chaotic case is only obtained if the N exceeds a certain threshold, $N \geq N_{thr} = 100$.
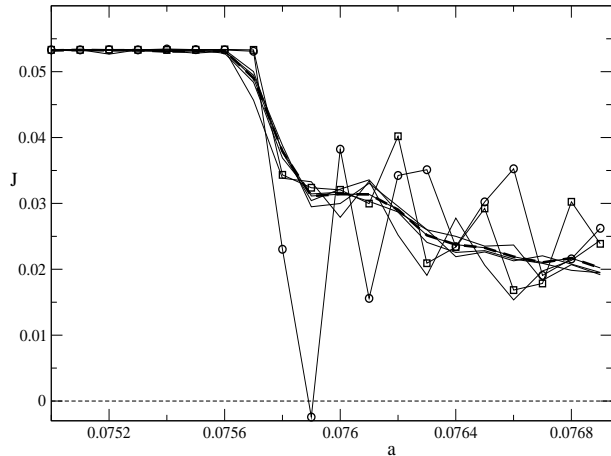

FIG. 3: Current J versus a for different set of trajectories N; $N = 1$ (circles), $N = 10$ (square) and $N = 100$ (dashed lines). Note that a single trajectory suffices in the regular regime where all the curves match. In the chaotic regime, as N increases, the curves converge towards the dashed one.

Also, note that single-trajectory current values are typically significantly greater than ensemble averages. This arises from the fact that an arbitrarily chosen ensemble has particles with idiosyncratic behaviors which often average out. As our result, with these ensembles we see typical $J \approx 0.01$ for example, while Barbi and Salerno

report currents about 10 times greater. However, it is not true that only a few trajectories dominate the dynamics completely, else there would not be a saturation of the current as a function of N. All this is clear in Fig. (3). We note that the **net** drift of an ensemble can be a lot closer to 0 than the behavior of an individual trajectory.

It should also be clear that there is a dependence of the current on the location of the initial ensemble, this being particularly true for small N, of course. The location is defined by its centroid $\langle x \rangle, \langle p \rangle$. For $N = 1$, it is trivially true that the initial location matters to the asymptotic value of the time-averaged velocity, given that this is a non-ergodic and chaotic system. Further, considering a Gaussian ensemble, say, the width of the ensemble also affects the details of the current, and can show, for instance, illusory current reversal, as seen in Figs. (6,7) for example. Notice also that in Fig. (6), at $a \approx 0.065$ and $a \approx 0.15$, the deviations between the different ensembles is particularly pronounced. These points are close to bifurcation points where some sort of symmetry breaking is clearly occuring, which underlines our emphasis on the relevance of specifying ensemble characteristics in the neighborhood of unstable behavior. However, why these specific bifurcations should stand out among all the bifurcations in the parameter range shown is not entirely clear.

To understand how to incorporate this knowledge into calculations of the current, therefore, consider the fact that if we look at the classical phase space for the Hamiltonian or underdamped ($b = 0$) motion, we see the typical structure of stable islands embedded in a chaotic sea which have quite complicated behavior[12]. In such a situation, the dynamics always depends on the location of the initial conditions. However, we are not in the Hamiltonian situation when the damping is turned on – in this case, the phase-space consists in general of attractors. That is, if transient behavior is discarded, the current is less likely to depend significantly on the location of the initial conditions or on the spread of the initial conditions.

In particular, in the chaotic regime of a non-Hamiltonian system, the initial ensemble needs to be chosen larger than a certain threshold to ensure convergence. However, in the regular regime, it is not important to take a large ensemble and a single trajectory can suffice, as long as we take care to discard the transients. That is to say, in the computation of currents, the definition of the current needs to be modified to:

$$J = \frac{1}{M - n_c} \sum_{j=n_c}^{M} v_j \qquad (5)$$

where n_c is some empirically obtained cut-off such that we get a converged current (for instance, in our calculations, we obtained converged results with $n_c = 1000, M = 20000$). When this modified form is used, the convergence (ensemble-independence) is more rapid as a function of N, M and the width of the intial conditions.

Armed with this background, we are now finally in a position to compare bifurcation diagrams with the current, as we do in the next section.

IV. THE RELATIONSHIP BETWEEN BIFURCATION DIAGRAMS AND ENSEMBLE CURRENTS

Our results are presented in the set of figures Fig. (4) – Fig. (9), in each of which we plot both the ensemble current and the bifurcation diagram as a function of the parameter a. The main point of these numerical results can be distilled into a series of heuristic statements which we state below; these are labelled with Roman numerals.
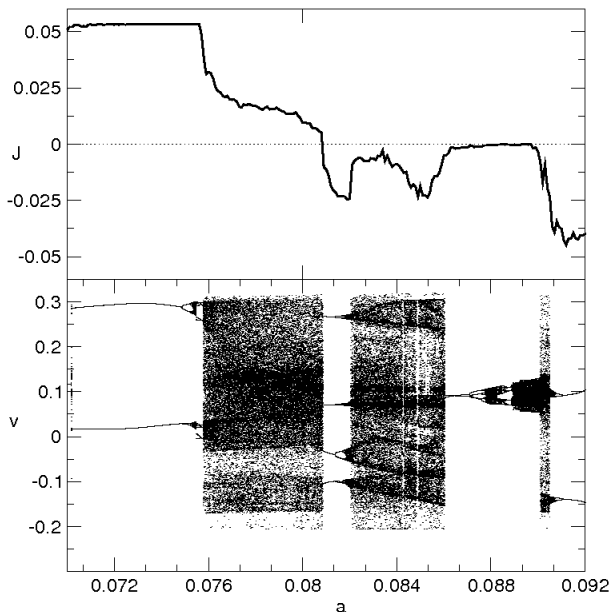
FIG. 4: For $\omega = 0.67$ and $b = 0.1$, we plot current (upper) with $N = 1000$ and bifurcation diagram (lower) versus a. Note that there is a **single** current reversal while there are many bifurcations visible in the same parameter range.

Consider Fig. (4), which shows the parameter range $a = \{0.07, 0.094\}$ chosen relatively arbitrarily. In this figure, we see several period-doubling bifurcations leading to order-chaos transitions, such as for example in the approximate ranges $a = \{0.075, 0.076\}, \{0.08, 0.082\}, \{0.086, 0.09\}$. However, there is only one instance of current-reversal, at $a \approx 0.08$. Note, however, that the current is not without structure – it changes fairly dramatically as a function of parameter.

This point is made even more clearly in Fig. (5) where the current remains consistently below 0, and hence there are in fact, no current reversals at all. Note again, however, that the current has considerable structure, even while remaining negative. It is possible to find several examples of this at different parameters, leading to the negative conclusion, therefore, that **(i) not all bifur-**
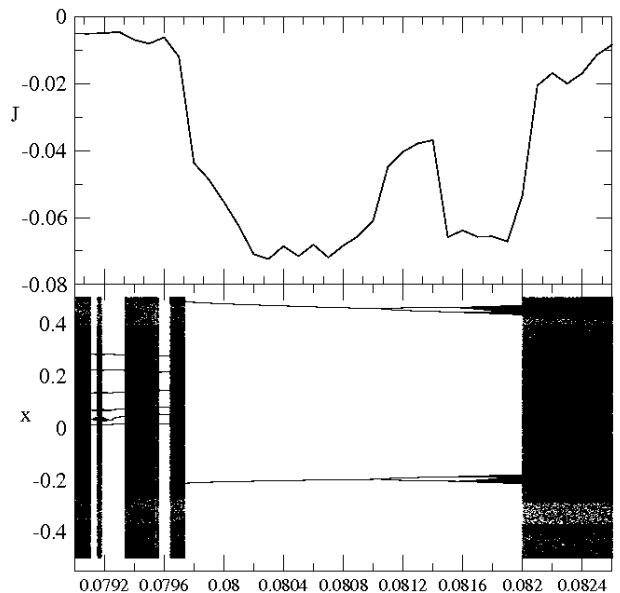

FIG. 5: For $\omega = 0.603$ and $b = 0.1$, plotted are current (upper) and bifurcation diagram (lower) versus a with $N = 1000$. Notice the current stays consistently below 0.

cations lead to current reversal. However, we are searching for positive correlations, and at this point we have not precluded the more restricted statement that all current reversals are associated with bifurcations, which is in fact Mateos' conjecture.

We therefore now move onto comparing our results against the specific details of Barbi and Salerno's treatment of this conjecture. In particular, we look at their Figs. (2,3a,3b), where they scan the parameter region $b = 0.1, \omega = 0, 67, a = \in (0.0, 0.24)$. The distinction between their results and ours is that we are using *ensembles* of particles, and are investigating the convergence of these results as a function of number of particles N, the width of the ensemble in phase-space, as well as transience parameters n_c, M.

Our data with larger N yields different results in general, as we show in the recomputed versions of these figures, presented here in Figs. (6,7). Specifically, (a) the single-trajectory results are, not surprisingly, cleaner and can be more easily interpreted as part of transitions in the behavior of the stability properties of the periodic orbits. The ensemble results on the other hand, even when converged, show statistical roughness. (b) The ensemble results are consistent with Barbi and Salerno in general, although disagreeing in several details. For instance, (c) the bifurcation at ($a \approx 0.07$) has a much gentler impact on the ensemble current, which has been growing for a while, while the single-trajectory result changes abruptly. Note, (d) the very interesting fact that the single-trajectory current completely misses the bifurcation-associated spike at ($a \approx 0.11$). Further, (e) the Barbi and Salerno discussion of the behavior of the current in the range $a \in (0.14, 0.18)$ is seen to be flawed
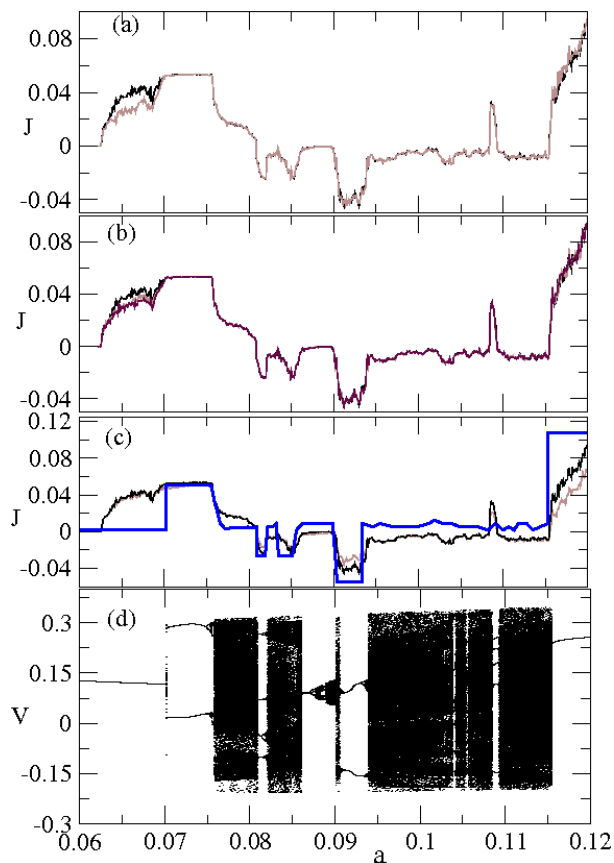
FIG. 6: Current and bifurcations versus a. In (a) and (b) we show ensemble dependence, specifically in (a) the black curve is for an ensemble of trajectories starting centered at the stable fixed point $(0,0)$ with a root-mean-square Gaussian width of 0.25, and the brown curve for trajectories starting from the unstable fixed point $(-0.375, 0)$ and of width 0.25. In (b), all ensembles are centered at the stable fixed point, the black line for an ensemble of width 0.25, brown a width of 0.5 and maroon with width 1.0. (c) is the comparison of the current J without transients (black) and with transients (brown) along with the single-trajectory results in blue (after Barbi and Salerno). The initial conditions for the ensembles are centered at $(0,0)$ with a mean root square gaussian of width 0.25. (d) is the corresponding bifurcation diagram.

– our results are consistent with theirs, however, the current changes are seen to be consistent with bifurcations despite their statements to the contrary. On the other hand (f), the ensemble current shows a case [in Fig. (7), at $a > 0.2$] of current reversal that does not seem to be associated with bifurcations. In this spike, the current abruptly drops below 0 and then rises above it again. The single trajectory current completely ignores this particular effect, as can be seen. The bifurcation diagram indicates that in this case the important transitions happen either before or after the spike.

All of this adds up to two statements: The first is a reiteration of the fact that there is significant information in the ensemble current that cannot be obtained from the single-trajectory current. The second is that the heuristic that arises from this is again a negative conclusion, that **(ii) not all current reversals are associated with bifurcations.** Where does this leave us in the search for 'positive' results, that is, useful heuristics? One possible way of retaining the Mateos conjecture is to weaken it, i.e. make it into the statement that **(iii) *most* current reversals are associated with bifurcations.**
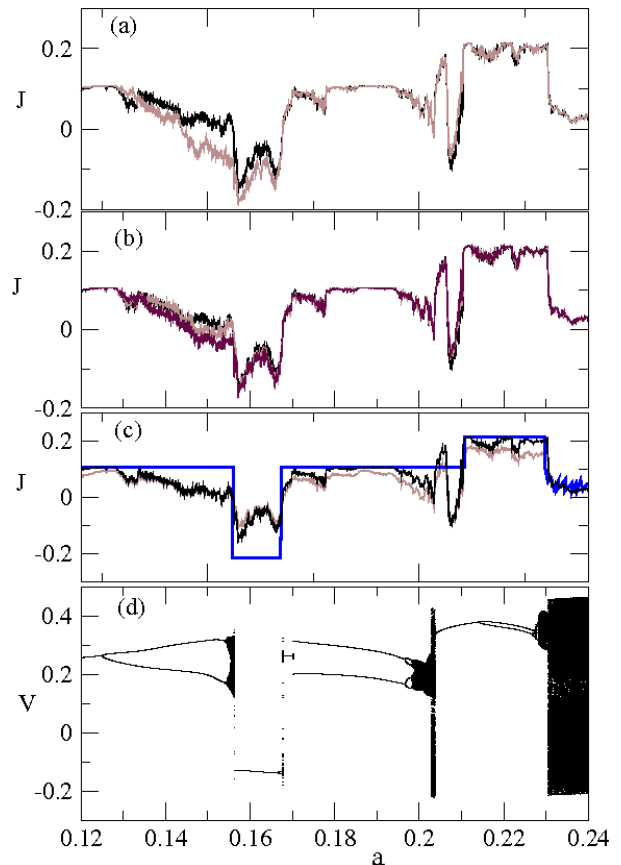

FIG. 7: Same as Fig. (6) except for the range of a considered.

However, a **different** rule of thumb, previously not proposed, emerges from our studies. This generalizes Mateos' conjecture to say that **(iv) bifurcations correspond to sudden current changes (spikes or jumps)**. Note that this means these changes in current are not necessarily reversals of direction. If this current jump or spike goes through zero, this coincides with a current reversal, making the Mateos conjecture a special case. The physical basis of this argument is the fact that ensembles of particles in chaotic systems *can* have net directed transport but the details of this behavior depends relatively sensitively on the system parameters. This parameter dependence is greatly exaggerated at the bifurcation point, when the dynamics of the underlying single-particle system undergoes a transition – a period-doubling transition, for example, or one from chaos to regular behavior. Scanning the relevant figures, we see that this is a very useful rule of thumb. For example, it
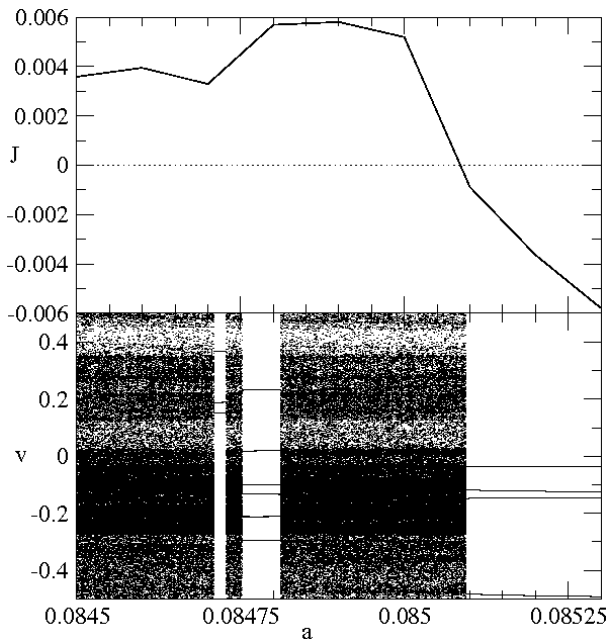
FIG. 8: For $\omega = 0.6164$ and $b = 0.1$, plotted are current (upper) and bifurcation diagram (lower) versus a with $N = 1000$. Note in particular in this figure that eyeball tests can be misleading. We see reversals without bifurcations in (a) whereas the zoomed version (c) shows that there are windows of periodic and chaotic regimes. This is further evidence that jumps in the current correspond in general to bifurcation.

FIG. 9: For $\omega = 0.67$ and $b = 0.11$, current (upper) and bifurcation diagram (lower) versus a.

completely captures the behaviour of Fig. (5) which cannot be understood as either an example of the Mateos conjecture, or even a failure thereof. As such, this rule significantly enhances our ability to characterize changes in the behavior of the current as a function of parameter.

A further example of where this modified conjecture helps us is in looking at a seeming negation of the Mateos conjecture, that is, an example where we seem to see current-reversal without bifurcation, visible in Fig. (8). The current-reversals in that scan of parameter space seem to happen inside the chaotic regime and seemingly independent of bifurcation. However, this turns out to be a 'hidden' bifurcation – when we zoom in on the chaotic regime, we see hidden periodic windows. This is therefore consistent with our statement that sudden current changes are associated with bifurcations. Each of the transitions from periodic behavior to chaos and back provides opportunities for the current to spike.

However, in not all such cases can these hidden bifurcations be found. We can see an example of this in Fig. (9). The current is seen to move smoothly across $J = 0$ with seemingly no corresponding bifurcations, even when we do a careful zoom on the data, as in Fig. (8). However, arguably, although subjective, this change is 'close' to the bifurcation point. This result, that there are situations where the heuristics simply do not seem to apply, are part of the open questions associated with this problem, of course. We note, however, that we have seen that these
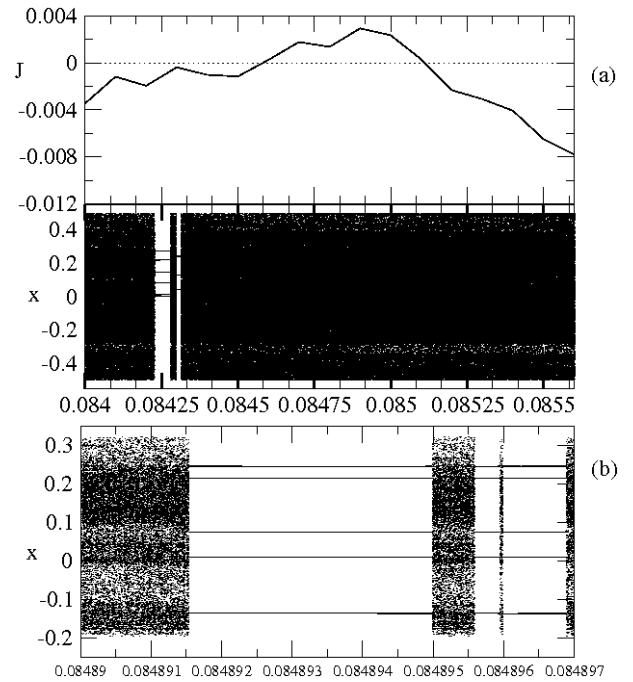
broad arguments hold when we vary other parameters as well (figures not shown here).

In conclusion, in this paper we have taken the approach that it is useful to find general rules of thumb (even if not universally valid) to understand the complicated behavior of non-equilibrium nonlinear statistical mechanical systems. In the case of chaotic deterministic ratchets, we have shown that it is important to factor out issues of size, location, spread, and transience in computing the 'current' due to an ensemble before we search for such rules, and that the dependence on ensemble characteristics is most critical near certain bifurcation points. We have then argued that the following heuristic characteristics hold: Bifurcations in single-trajectory behavior often corresponds to sudden spikes or jumps in the current for an ensemble in the same system. Current reversals are a special case of this. However, not all spikes or jumps correspond to a bifurcation, nor vice versa. The open question is clearly to figure out if the reason for when these rules are violated or are valid can be made more concrete.

V. ACKNOWLEDGEMENTS

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